Journal of Molecular Structure (Theochem), 234 (1991) 539
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Ågren, H., 425
Alcamí, M., 357

Bader, R.F.W., 75
Barnett, R.N., 525
Basch, H., 185
Bloor, J.E., 173
Bock, C.W., 227
Bonaccorsi, R., 401

Cammi, R., 401
Cremer, D., 95

Deakyne, C.A., 343
Del Bene, J.E., 499
Demel, K., 329
Disch, R.L., 213
Duch, W., 27

Eckert-Maksić, M., 201

Gauss, J., 95
Geerlings, P., 329
George, P., 227
Glusker, J.P., 227
Greenberg, A., 291

Ha, T.-K., 515
Hall, G.G., 13
Hammond, B.L., 525
Hodošček, M., 201

Hutter, J., 515
Huzinga, S., 51

Janoschek, R., 509

Kalcher, J., 509
Keefe, C.D., 19
Kovaček, D., 201
Kraka, E., 95
Kudnig, J., 201

Laidig, K.E., 75
Langenaeker, W., 329
Latajka, Z., 373
Lazzeretti, P., 127
Leroy, G., 303
Lester, W.A., Jr., 525
Liebman, J.F., 343
Lüthi, H.P., 515

Maksić, Z.B., 201
Malagoli, M., 127
Mikkelsen, K.V., 425
Mizukami, Y., 469
Mó, O., 357

Nakatsuji, H., 469
Nicolaides, C.A., 483

Olivares del Valle, F.J., 401

Plant, C., 291
Poirier, R.A., 19
Poljanec, K., 201
Pyykkö, P., 269, 279

Roothaan, C.J., 1
Roszak, S.M., 387
Runeberg, N., 269, 279

Sadlej, A.J., 147
Sana, M., 303
Schaefer, H.F. III, 247
Scheiner, S., 373
Schulman, J.M., 213
Shavitt, I., 499
Sokalski, W.A., 387
Soto, M.M., 525

Thrasher, J.S., 247
Tomasi, J., 401

Urban, M., 147

Valtazanos, P., 483
Venanzi, C.A., 291

Wilante, C., 303

Xie, Y., 247

Yáñez, M., 357

Zanasi, R., 127

Journal of Molecular Structure (Theochem), 234 (1991) 541–543
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

$A=B-C=D^n$ and $A=B=C=D^n$ systems
Ab initio studies of bonding trends. Part 8. The 26-electron $A=B-C=D^n$ and the 30-electron $A=B=C=D^n$ systems, 269
A=B=C=D=E isoelectronic series
Ab initio studies of bonding trends. Part 9. The dicyanamide–carbon suboxide–dicyanoether–cyanogen azide isoelectronic series A=B=C=D=E, 279
Al^+ complexes
An ab initio molecular orbital study of the structure, energetics and bond activation of Al^+ complexes, 357
Alkali atoms
Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties. III. Alkali (Li, Na, K, Rb) and alkaline-earth (Be, Mg, Ca, Sr) atoms, 147
Alkaline-earth atoms
Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties. III. Alkali (Li, Na, K, Rb) and alkaline-earth (Be, Mg, Ca, Sr) atoms, 147
Anionic bases
The relative Lewis acidities of BF_3 and SO_3: the enthalpies of complexation with the anionic bases F^-, OH^-, NH_2^-, CH_3^- and CF_3^-, 343
[18]Annulene
On the structure and thermochemistry of [18] annulene, 213
Aromaticity
The conjunction of aromaticity and hypervalency: the $C_5H_5SF_3$ molecule, 1,1,1-trifluorothiabenzene, 247
Atoms in molecules
The prediction and calculation of properties of atoms in molecules, 75

Benzene molecule
Coupled Hartree–Fock calculations of magnetic properties of the benzene molecule: estimate of the Hartree–Fock limit for magnetic susceptibilities and nuclear shieldings, 127

BF_3
The relative Lewis acidities of BF_3 and SO_3: the enthalpies of complexation with the anionic bases F^-, OH^-, NH_2^-, CH_3^- and CF_3^-, 343
Bonding trends
Ab initio studies of bonding trends. Part 8. The 26-electron $A=B-C=D^n$ and the 30-electron $A=B=C=D^n$ systems, 269
Bonding trends
Ab initio studies of bonding trends. Part 9. The dicyanamide–carbon suboxide–dicyanoether–cyanogen azide isoelectronic series A=B=C=D=E, 279

C_3 in the CASSCF approach
Electronically excited states of C_3 in the CASSCF approach, 509
Closed-shell systems
The influence of *gem*-substitution on the stability of open-shell and closed-shell systems. The captodative and anomeric effects re-examined, 303
Computational quantum chemistry
Computational quantum chemistry — then and now, 13
Configuration interaction method
Configuration interaction method: the past and future perspectives, 27
Correlated proton transfer potentials
Correlated proton transfer potentials. $(HO-H-OH)^-$ and $(H_2O-H-OH_2)^+$, 373

Electronic spectra
Theory of solvent effects on electronic spectra, 425
Electronic structure of molecules
On quantum Monte Carlo for the electronic structure of molecules, 525
Electronic structure studies
Geometry and electronic structure studies using computational quantum chemistry, 185

Fukui function
Quantum-chemical study of the Fukui

function as a reactivity index. Part 2. Electrophilic substitution on mono-substituted benzenes, 329

Gem-substitution
The influence of *gem*-substitution on the stability of open-shell and closed-shell systems. The captodative and anomeric effects re-examined, 303

Geometry studies
Geometry and electronic structure studies using computational quantum chemistry, 185

$(H_2O)_2^*$ cluster
The $(H_2O)_2^*$ cluster at a geometry of intramolecular charge transfer, 483

Hamiltonian method
Effective Hamiltonian method for molecules, 51

Hartree–Fock limit
Coupled Hartree–Fock calculations of magnetic properties of the benzene molecule: estimate of the Hartree–Fock limit for magnetic susceptibilities and nuclear shieldings, 127

HCl trimers
A theoretical study of the neutral, protonated, and deprotonated trimers of HF and HCl, 499

HF trimers
A theoretical study of the neutral, protonated, and deprotonated trimers of HF and HCl, 499

HOOH
Ab initio CI calculation of the electronic states of HOOH: oscillator strengths and optical rotatory strengths, 515

Hypervalency
The conjunction of aromaticity and hypervalency: the $C_5H_5SF_3$ molecule 1,1,1-trifluorothiabenzene, 247

Intermolecular interaction energy
Efficient techniques for the decomposition of intermolecular interaction energy at SCF level and beyond, 387

Kr_2 ionized states
Potential energy curves of the 5s Rydberg excited states and ionized states of Kr_2 studied by the SAC–CI theory, 469

Magnetic susceptibilities
Coupled Hartree–Fock calculations of magnetic properties of the benzene molecule: estimate of the Hartree–Fock limit for magnetic susceptibilities and nuclear shieldings, 127

1-Methylsilatrane and model compounds
Ab initio molecular orbital study of 1-methylsilatrane and model compounds, 291

Mills–Nixon effect
Is the Mills–Nixon effect operative in perfluoro-benzo[1,2:3,4:5,6]tricyclobutene?, 201

Molecular electric properties
Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties. III. Alkali (Li, Na, K, Rb) and alkaline-earth (Be, Mg, Ca, Sr) atoms, 147

Mono-substituted benzenes
Quantum-chemical study of the Fukui function as a reactivity index. Part 2. Electrophilic substitution on mono-substituted benzenes, 329

Naphthalene
A computational molecular orbital study of the oxide and oxepin valence tautomers of naphthalene, 227

Nuclear shieldings
Coupled Hartree–Fock calculations of magnetic properties of the benzene molecule: estimate of the Hartree–Fock limit for magnetic susceptibilities and nuclear shieldings, 127

Open-shell systems
The influence of *gem*-substitution on the stability of open-shell and closed-shell systems. The captodative and anomeric effects re-examined, 303

Perfluoro-benzo[1,2:3,4:5,6]tricyclobutene
Is the Mills–Nixon effect operative in perfluoro-benzo[1,2:3,4:5,6]tricyclobutene?, 201

Response densities
Determination and use of response densities, 95
5s Rydberg excited states
Potential energy curves of the 5s Rydberg excited states and ionized states of Kr_2 studied by the SAC–CI theory, 469

SCF calculations
Computational developments in SCF calculations, 19
SO_3
The relative Lewis acidities of BF_3 and SO_3: the enthalpies of complexation with the anionic bases F^-, OH^-, NH_2^-, CH_3^- and CF_3^-, 343
Solvent effects
Theory of solvent effects on electronic spectra, 425

Theoretical chemistry in solution
Theoretical chemistry in solution. Some results and perspectives of the continuum methods and in particular of the polarizable continuum model, 401
1,1,1-Trifluorothiabenzene
The conjunction of aromaticity and hypervalency: the $C_5H_5SF_3$ molecule, 1,1,1-trifluorothiabenzene, 247

Water molecule
Finite field ab initio calculations of the dipole polarizabilities and first and second hyperpolarizabilities using multiple sets of polarization functions. I. The water molecule, 173